



chain nodes :

13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 34

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12

chain bonds :

2-25 5-13 9-13 12-18 13-14 13-16 14-15 16-17 18-19 18-20 19-21 21-22 22-23 22-24
23-34 25-26 26-27 27-28 27-29 29-30 29-31 29-32

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

exact/norm bonds :

2-25 18-19 18-20 19-21 22-23 22-24 23-34 25-26 27-28

exact bonds :

5-13 9-13 12-18 13-14 13-16 14-15 16-17 21-22 26-27 27-29 29-30 29-31 29-32

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

isolated ring systems :

containing 1 : 7 :

G1:N,Hy,Ak,H

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS
21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS
30:CLASS 31:CLASS 32:CLASS 34:CLASS